

The BCS Pairing Instability in the Thermodynamic Limit

F. Marsiglio,¹ K. S. D. Beach,¹ and R. J. Gooding²

¹*Department of Physics, University of Alberta, Edmonton, Alberta, Canada, T6G 2E1*

²*Department of Physics, Engineering Physics and Astronomy, Queen's University, Kingston ON K7L 3N6*

(Dated: March 1, 2013)

The superconducting pairing instability—as determined by a divergence of the two-particle susceptibility—is obtained in the mean field (BCS) approximation in the thermodynamic limit. The usual practice is to examine this property for a finite lattice. We illustrate that, while the conclusions remain unchanged, the technical features are very different in the thermodynamic limit and conform more closely with the usual treatment of phase transitions encountered in, for example, the mean-field paramagnetic-ferromagnetic transition. Furthermore, by going to the extreme dilute limit, one can distinguish three dimensions from one and two dimensions, in which a pairing instability occurs even for two particles.

I. INTRODUCTION

The Bardeen, Cooper, and Schrieffer (BCS) theory of superconductivity, following the original literature,¹ is typically first presented in textbooks as a proposed variational ground state, whose energy is lower than that of the corresponding normal state.^{2,3} This is followed by a discussion of the excited states, from which, in weak coupling at least, a critical temperature is derived, corresponding to the breakup of pairs.

An alternate view of the transition was put forward by Thouless,⁴ who tracked the BCS instability from above (in temperature) by monitoring the two particle propagator. By including a specific set of processes (denoted by “ladders” in the particle-particle channel of the diagrammatic version of this formulation), one finds an instability of the normal phase. This approach is also explained in many texts^{2,5} and will be briefly summarized below.

Seeing the superconducting transition as an instability of the normal state at some finite temperature highlights the potential importance of pairing fluctuations that occur in the normal state even before the critical transition is reached. The possibility of pairing fluctuations has been important in the elucidation of the so-called pseudo-gap that occurs in the high- T_c cuprate materials. One school of thought regards the pseudo-gap in these materials as a tell-tale signature of pairing fluctuations in the normal state.⁶

There is now an extensive literature on the presence of pairing fluctuations in the normal state and on their impact on various normal state properties.^{7–9} However, our purpose here is to revisit the simple so-called Thouless criterion for the BCS instability and to reformulate it in the thermodynamic limit. We have always found it peculiar that this instability is signalled by the appearance of two *imaginary* roots in the denominator of the two-particle propagator, whereas other instabilities appear to be accompanied by the appearance of a *real* root.¹⁰ It turns out that the two-particle pairing instability is always, to our knowledge, formulated for a finite system; in the thermodynamic limit, as we show below, the criterion behaves quite differently and much more like

other instabilities in condensed matter.

For simplicity we focus on the simplest model that exhibits superconductivity (at least at the mean field level), the attractive Hubbard model on a hypercubic lattice in one, two, and three dimensions.¹¹ While considerable attention has been devoted to single-particle properties, since these are often most related to the measured properties,⁶ the two-particle properties are the ones that are key to understanding single-particle properties.¹² For our purposes, we express the two-particle propagator in the non-self-consistent ladder approximation,¹¹

$$g_2(\mathbf{q}, i\nu_n) \equiv \frac{\chi_0(\mathbf{q}, i\nu_n)}{1 - |U|\chi_0(\mathbf{q}, i\nu_n)}, \quad (1)$$

where χ_0 is the “noninteracting” pair susceptibility

$$\chi_0(\mathbf{q}, i\nu_n) = \frac{1}{N\beta} \sum_{\mathbf{k}, m} G_{0\uparrow}(\mathbf{k}, i\omega_m) G_{0\downarrow}(\mathbf{q} - \mathbf{k}, i\nu_n - i\omega_m), \quad (2)$$

and $G_{0\sigma}(\mathbf{k}, i\omega_m) = [i\omega_m - (\epsilon_{\mathbf{k}} - \mu)]^{-1}$ is the noninteracting single-particle propagator. Here, \mathbf{k} and \mathbf{q} are wave vectors, and $\epsilon_{\mathbf{k}}$ is the single electron dispersion appropriate to tight-binding with nearest neighbour hopping. The Matsubara frequencies are defined as $i\omega_m \equiv \pi T(2m - 1)$ for Fermions and $i\nu_n \equiv i2\pi Tn$ for Bosons. $\beta \equiv (k_B T)^{-1}$ is the inverse temperature, and N is the number of lattice sites. All wavevector summations span the entire Brillouin zone, and Matsubara sums go over all integers.

For the BCS instability we can focus on $\mathbf{q} = 0$ and, in fact, $\nu_n = 0$; nonetheless, we wish to illustrate the instability by monitoring g_2 as a function of (real) frequency. The result for χ_0 is

$$\chi_0(\mathbf{q}, z) = -\frac{1}{N} \sum_{\mathbf{k}} \frac{1 - f(\epsilon_{\mathbf{k}} - \mu) - f(\epsilon_{-\mathbf{k}+\mathbf{q}} - \mu)}{z - (\epsilon_{\mathbf{k}} - \mu) - (\epsilon_{-\mathbf{k}+\mathbf{q}} - \mu)}, \quad (3)$$

where we have now analytically continued the result to the upper half-plane ($i\nu_n \rightarrow z$), and in particular for $z = \nu + i\delta$, with δ a positive infinitesimal. Here $f(x) \equiv 1/(e^{\beta x} + 1)$ is the Fermi-Dirac distribution function. Equation (3) is the one displayed in textbooks and reviews. We show its real and imaginary parts in

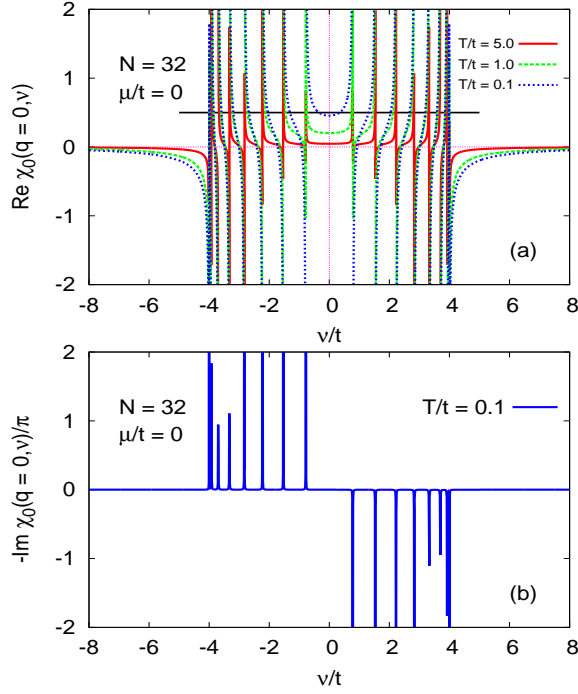


FIG. 1. Real (a) and Imaginary (b) parts of the noninteracting pair susceptibility at zero wave vector vs. frequency, for three different temperatures. Note that poles occur at the energies corresponding to two single electron energies. In addition, the minimum at zero frequency diverges as the temperature goes to zero (not evident in (a) because the divergence is logarithmic). The figures were produced in one dimension with a finite lattice of length 32 sites. The horizontal line at 0.5 in (a) denotes the value of $1/|U|$ for $|U| = 2t$. As the central minimum rises above this horizontal line (with decreasing temperature) an instability is signalled, as discussed in the text.

Fig. 1, for a finite (1D) system with $N = 32$ at half-filling ($\mu = 0$) and for a number of temperatures. The chemical potential can either be held fixed or tuned to produce a desired electron density, n .

The use of a finite lattice necessarily produces a series of poles, as is evident in Fig. 1(b), where the imaginary part of χ_0 is plotted (a small numerical value of δ is used in place of an infinitesimal). These poles correspond to the noninteracting case ($|U| = 0$); they arise from roots of the denominator in Eq. (3) with a small *negative* imaginary part and hence lie in the lower half plane. This fact renders them “innocent,” since, when substituted into the original time-dependent propagator, $e^{-i\nu t}$, they will decay away with time. They correspond to normal two-particle excitations and result in a density of states that extends across the two-particle continuum. In this one dimensional case, these energies extend from twice the energy of the bottom of the band ($-4t$) to twice the energy of the top of the band ($4t$). At high temperatures the excitation energies occur at energies very close to those of the noninteracting case, indicated by the ver-

tical asymptotes in Fig. 1(a); in this case the energies are all slightly shifted by the interaction and occur not at the asymptotes but at the intersection of the curve with the horizontal black line, representing $1/|U|$. These intersections correspond to the zeros of the denominator in Eq. (1) and will be referred to as the poles of the two-particle propagator.

A special case, with a distinctive temperature dependence, is the pair of zeros near $\nu = 0$. As the temperature decreases, the zero frequency minimum in Fig. 1(a) increases in value and eventually crosses $1/|U|$. As it does so, two real roots (with small negative imaginary part) become two pure imaginary roots, one of which is in the upper half plane. Substitution of this root into $e^{-i\nu t}$ results in an excitation that blows up with time, indicative of an unstable normal phase.^{2,5,13}

We now outline the situation in the thermodynamic limit, which, while giving the same physics, looks quite different. For $\mathbf{q} = 0$ the discrete sum in Eq. (3) is converted to an integral over the single-particle density of states, $g(\epsilon)$.¹⁴

$$\chi_0(\nu + i\delta) = - \int_{-W/2}^{+W/2} d\epsilon g(\epsilon) \frac{\tanh(\beta(\epsilon - \mu)/2)}{\nu + i\delta - 2(\epsilon - \mu)}, \quad (4)$$

where $\pm W/2$ is the top (bottom) of the single electron band ($\pm 2t$ in 1D, $\pm 4t$ in 2D, and $\pm 6t$ in 3D), and since $\mathbf{q} = 0$ we have omitted it from the argument list for χ_0 . This integral requires a principal value part, which can be done analytically:

$$\begin{aligned} \chi_0(\nu + i\delta) = & \frac{1}{2} g\left(\frac{\nu}{2} + \mu\right) \tanh \frac{\beta\nu}{4} \log \left\{ \frac{\frac{W}{2} - \mu - \frac{\nu + i\delta}{2}}{\frac{W}{2} + \mu + \frac{\nu + i\delta}{2}} \right\} \\ & + i \frac{\pi}{2} g\left(\frac{\nu}{2} + \mu\right) \tanh \frac{\beta\nu}{4} \\ & + \frac{1}{2} \int_{-W/2}^{+W/2} d\epsilon \frac{g(\epsilon) \tanh \frac{\beta(\epsilon - \mu)}{2} - g\left(\frac{\nu}{2} + \mu\right) \tanh \frac{\beta\nu}{4}}{\epsilon - \mu - (\nu + i\delta)/2}. \end{aligned} \quad (5)$$

The integration on the last line is no longer singular and can be computed by quadrature.

In Figs. 2(a) and 2(b) we show the corresponding results for an infinite system (in 1D) at temperatures $T = 1, 0.1$, and 0.01 (in units of t ; hereafter all energies will be quoted in units of t). The real part of $\chi_0(\nu)$ clearly shows a *maximum* at zero frequency; elsewhere there are no positive divergences as they have been integrated to a smooth curve in the principal value sense. The negative divergences occur at the band edges and are due to the divergent single electron density of states at the band edges in one dimension.

As is apparent from the figure, these “band edge” divergences are present at all temperatures. In fact, for the lowest two temperatures shown, the curves are essentially the same *except for the region near zero frequency*, where the maximum diverges as $T \rightarrow 0$, indicative of a superconducting/charge-density-wave instability. In fact

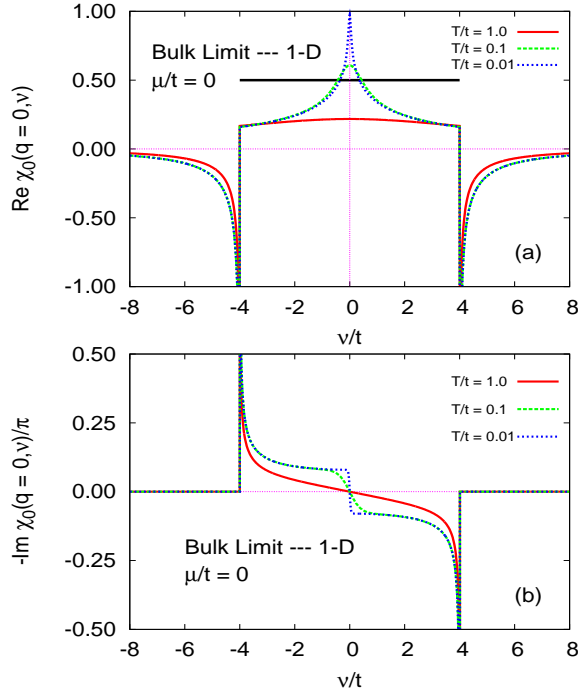


FIG. 2. Real (a) and Imaginary (b) parts of the noninteracting susceptibility at zero wavevector vs. frequency, for three different temperatures, for the bulk limit in one dimension. Note that part (a) in particular looks very different from the finite size counterpart in Fig. (1a). In particular, the poles corresponding to sums of single electron energies are evident only in (b). The developing singularity at zero frequency remains, as is evident in (a).

at zero temperature the real part is given analytically by the following expression (for $\mu = 0$):

$$\text{Re } \chi_0(\nu + i\delta) = \begin{cases} \frac{1}{4\pi t} \frac{1}{\sqrt{1-\bar{\nu}^2}} \log \left(\frac{1+\sqrt{1-\bar{\nu}^2}}{1-\sqrt{1-\bar{\nu}^2}} \right) & \bar{\nu} < 1, \\ -\frac{1}{2\pi t} \frac{1}{\sqrt{\bar{\nu}^2-1}} \arctan \left(\frac{1}{\sqrt{\bar{\nu}^2-1}} \right) & \bar{\nu} > 1, \end{cases} \quad (6)$$

where $\bar{\nu} \equiv \nu/(4t)$. The divergence at zero frequency is evident in this expression. At finite temperature an exact analytical expression is not possible, even for zero frequency. However, to a very good approximation one can obtain $\text{Re } \chi_0(\nu = 0) = \frac{1}{2\pi t} \log(1.13 \frac{4t}{T})$. Notice that the argument of the natural logarithm is a factor of 2 larger than what would have been obtained by simply approximating the density of states as a constant at the chemical potential ($\mu = 0$ in this case).

For a nonzero attractive interaction, an instability is signalled by the maximum crossing the black horizontal line positioned at $1/|U|$. This signals the onset of an instability in a way that is familiar from studies in mean-field ferromagnetism,¹⁰ for example. It *appears* as though two *real* roots are emerging; in fact a careful analysis of Eq. (1), using $\chi_0(\nu + i\delta) \approx a_0 + ic_0\nu$, with a_0 and c_0 positive real constants [see Figs. 2(a) and (b)] near $\nu \approx$

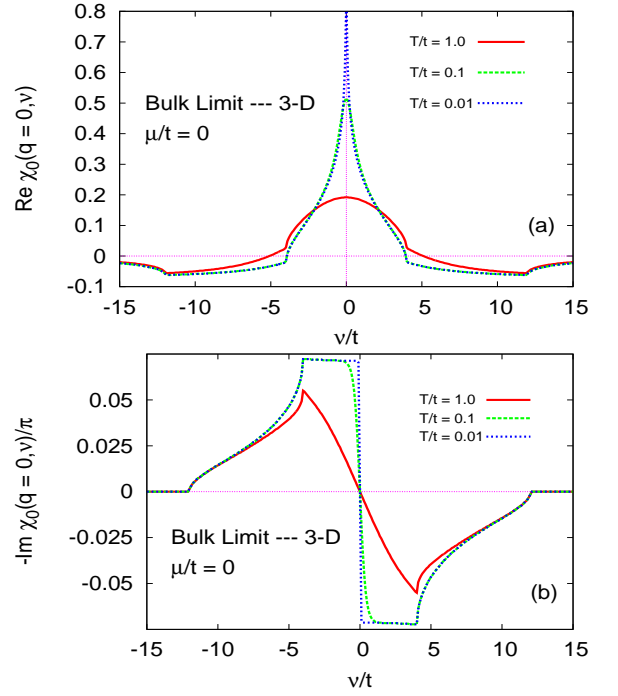


FIG. 3. Real (a) and Imaginary (b) parts of the noninteracting susceptibility at zero wavevector vs. frequency, for three different temperatures, for the bulk limit in three dimensions. In 3 dimensions no singularities occur at $\pm 12t$, since the single electron density of states starts smoothly from zero. The logarithmic divergence in temperature remains at zero frequency.

0 shows that as a_0 traverses $1/|U|$, the same root with *negative* imaginary part becomes a root with a *positive* imaginary part. As in the finite lattice case, then, the two particle propagator becomes unstable in time.

Figure (2b) shows the spectral function, $B_0(\mathbf{q}, \nu) \equiv -\text{Im } \chi_0(\mathbf{q}, \nu + i\delta)/\pi$ as a function of frequency. Aside from the asymmetrization, this quantity provides an image of the single electron density of states. This remains true in any dimension, as can be seen from taking the imaginary part of Eq. (5):

$$B_0(\mathbf{q} = 0, \nu) = -\frac{1}{2} \tanh\left(\frac{\beta\nu}{4}\right) g\left(\frac{\nu}{2} + \mu\right). \quad (7)$$

As the temperature approaches zero, the hyperbolic tangent function simply changes the sign of the density of states at the origin. In Fig. (1b) the delta function structure was merely providing an image of the finite system's discretized density of states.

As mentioned, this calculation can be done in any dimension, and Fig. (3a) and (3b) show the real and imaginary parts of the pair propagator in three dimensions, with nearest neighbour hopping only, at half filling. Once again the essential feature is that the real part diverges at zero frequency with decreasing temperature; thus, within mean field theory, Eq. (1) guarantees a transition when the real part crosses $1/|U|$. Of special note is the lack of

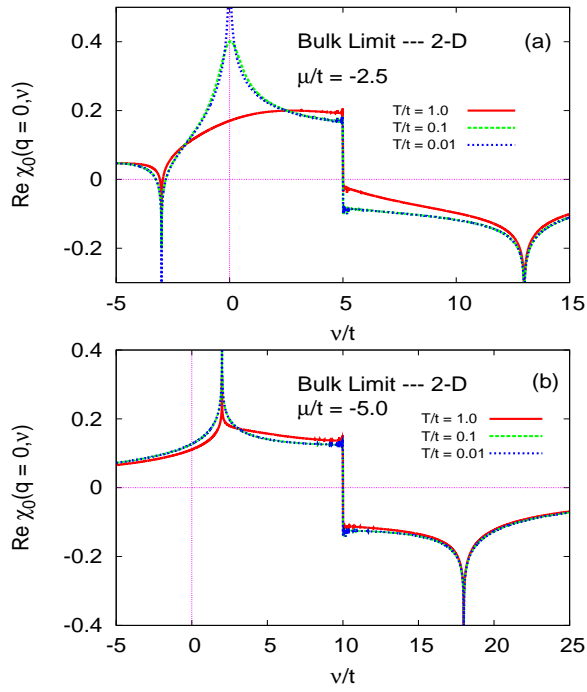


FIG. 4. Real part of the noninteracting susceptibility at zero wavevector vs. frequency, for three different temperatures, for the bulk limit in two dimensions, with nonzero chemical potential (a) above the bottom of the band, and (b) below the bottom of the band. The chemical potential in (a) ($\mu = -2.5t$) corresponds to some low filling of the band. Note that the divergence in the real part occurs again at $\nu = 0$, while the imaginary part of the susceptibility remains pinned to zero at this frequency. In contrast, the chemical potential in (b) ($\mu = -5.0t$) lies below the bottom of the band; this means that the real part of the susceptibility diverges at all temperatures, and signals a bound state being formed, even by two electrons. In 3D this does *not* occur for a single pair.

a negative divergence at the band edges in three dimensions; this affects the extreme dilute limit, and we will comment further below.

Finally, while half-filling gives rise to symmetric results, more often than not some other instability intervenes to suppress the pairing instability in this case. A result illustrating the pairing instability at a chemical potential away from half-filling is shown in Fig. 4, where the real part of the susceptibility is shown in two dimensions for (a) $\mu = -2.5t$ and (b) $\mu = -5.0$. Note that the divergence in the real part persists in (a) at $\nu = 0$ as the temperature is lowered. The negative divergences associated with the band edge discontinuities (in 1D and 2D) remain, but at a frequency $\pm W - 2\mu$. The discontinuity at $\nu = -2\mu$ ($5t$ for this case) is only present here because of the logarithmic divergence in the 2D density of states at the origin and is absent for other band structures that lack singularities. In (b) the chemical potential is below the bottom of the band; now there is a *positive* divergence at $\nu = -W - 2\mu$ (here at $2t$). This divergence

is peculiar to 2D and 1D only and shows that any $|U|$, no matter how small, will lead to an instability in the extreme dilute limit. This is *not* the case in higher dimension. For 3D, there is no band edge divergence, and it is well-known that an attractive potential must exceed some threshold before it will support a bound state for two particles.

Results in other dimensions away from half-filling are similar, albeit with differences reflecting the different densities of states, as already noted at half-filling, and the critical difference just noted regarding band edge divergences in 3D vs. 2D and 1D. Furthermore, completely symmetric results occur for $\mu = +2.5$ (compared to $\mu = -2.5$), due to the particle-hole symmetry in the problem.

In summary we have computed the two particle pairing susceptibility in the thermodynamic limit, in a variety of dimensions and for any filling. We have shown how the BCS instability comes about with decreasing temperature and how the nature of the instability more closely resembles the one usually discussed in the context of mean-field ferromagnetism. Technically, at the instability temperature, a single pole passes from the lower half-plane to the upper-half-plane in complex frequency. This is in contrast to the finite lattice result, where two real roots become two pure imaginary roots, one of which leads to the instability. In either case the change at the instability signals a two-particle propagator that diverges with increasing time.

The calculations in the thermodynamic limit enable one to see the dependence on dimensionality. Some quantitative differences occur due to the very different single-particle densities of states in 1D, 2D and 3D. However, in the extreme dilute limit, the different physics in 3D vs. 1D and 2D is highlighted in the thermodynamic limit, and leads, in a natural way, to the necessity in 3D for Cooper's famous calculation.¹⁵

ACKNOWLEDGMENTS

This work was supported in part by the Natural Sciences and Engineering Research Council of Canada (NSERC), and by the Canadian Institute for Advanced Research (CIFAR).

-
- ¹ J. Bardeen, L.N. Cooper and J.R. Schrieffer, Phys. Rev. **106**, 162 (1957); Phys. Rev. **108**, 1175 (1957).
- ² J.R. Schrieffer, *Theory of Superconductivity* (Benjamin/Cummings, Don Mills, 1964).
- ³ G. Rickayzen, *Theory of Superconductivity* (John Wiley and Sons, Inc. New York, 1965).
- ⁴ D.J. Thouless, Ann. Phys. **10**, 553 (1960). See also D.J. Thouless, *The Quantum Mechanics of Many-Body Systems*, (Academic Press, New York, 1961).
- ⁵ V. Ambegaokar, in *Superconductivity*, edited by R.D. Parks (Marcel Dekker, New York (1969)) Vol. 1, p.259.
- ⁶ T. Timusk and B. Statt, Rep. Prog. Phys. **62**, 61 (1999).
- ⁷ This perhaps started with Thouless,⁴ and was continued through the 1960's with Kadanoff and Baym and coworkers (L.P. Kadanoff and P.C. Martin, Phys. Rev **124**, 670 (1961), G. Baym and L.P. Kadanoff, Phys. Rev. **124**, 287 (1961), and G. Baym, Phys. Rev. **127** 1391 (1962)). Eagles (D. M. Eagles, Phys. Rev. **186**, 456 (1969)), Leggett (A.J. Leggett, J. de Physique, C7, **41**, 19 (1980); A.J. Leggett, in *Modern Trends in the Theory of Condensed Matter*, edited by S. Pekalski and J. Przystawa (Springer, Berlin, 1980)p. 13.) and eventually P. Nozières and S. Schmitt-Rink, J. Low Temp. Phys. **59**, 195 (1985), addressed the same issues, but posed the problem as a weak-strong (BCS-BEC) cross-over issue, and how best to capture effects omitted in the extreme (BCS or BEC) approaches.
- ⁸ References to work throughout the 1990's can be found in R.J. Gooding, F. Marsiglio, S. Verga, and K.S.D. Beach, J. Low Temp. Phys. **136**, 191 (2004).
- ⁹ A review with applications to cold atom lattices can be found in Q.J. Chen, J. Stajic, S. Tan, and K. Levin, Phys. Rep. **412**, 1 (2005).
- ¹⁰ For example, with the Stoner criterion for magnetism; see, for example, S. Doniach and E.H. Sondheimer, *Green's Functions for Solid State Physicists*, (Benjamin/Cummings, Don Mills, 1974).
- ¹¹ For notation, etc. see, for example, K.S.D. Beach, R.J. Gooding, and F. Marsiglio, Phys. Lett. A **282**, 319 (2001), and, more recently, S. Verga, R.J. Gooding, and F. Marsiglio, Phys. Rev. B **71**, 155111 (2005).
- ¹² This is most emphasized in the two-particle self-consistent approach of J. Vilk and A.-M.S. Tremblay, J. de Physique I (France) **7**, 1309 (1997). See also A.-M.S. Tremblay, B. Kyung and D. Senechal, Low. Temp. Phys. **32**, 424 (2006); [Fiz. Nizk. Temp. **32**, 561 (2006)].
- ¹³ See also Kadanoff and Martin in Ref. [7].
- ¹⁴ The single-particle densities of states are readily determined ahead of time for a hypercubic lattice in one, two, and three dimensions. See, for example, Appendix A in F. Marsiglio and J.E. Hirsch, Phys. Rev. B **41**, 6435 (1990).
- ¹⁵ L.N. Cooper, Phys. Rev. **104**, 1089 (1956).